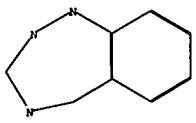
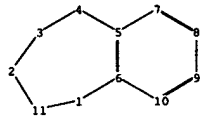
C:\Program Files\Stnexp\Queries\10655364.str





ring nodes :
1 2 3 4 5 6 7 8 9 10 11
ring bonds :
1-6 1-11 2-3 2-11 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10
exact/norm bonds :
1-6 1-11 2-3 2-11 3-4 4-5
normalized bonds :
5-6 5-7 6-10 7-8 8-9 9-10

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom

```
=> d his

     (FILE 'HOME' ENTERED AT 15:42:01 ON 08 FEB 2006)

     FILE 'REGISTRY' ENTERED AT 15:42:09 ON 08 FEB 2006
L1                STRUCTURE UPLOADED
L2              2 S L1
L3                STRUCTURE UPLOADED
L4              1 S L3
L5             41 S L3 SSS FUL

     FILE 'CAPLUS' ENTERED AT 15:43:28 ON 08 FEB 2006
L6              4 S L5

=> d l3
L3 HAS NO ANSWERS
L3                STR
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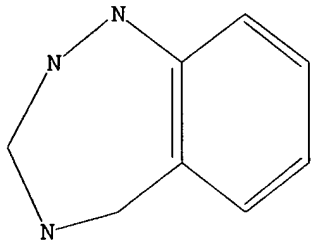

Structure attributes must be viewed using STN Express query preparation.

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=> d ibib abs hitstr total
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L6 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:203177 CAPLUS
DOCUMENT NUMBER: 140:235731
TITLE: Preparation of cinnolines and their use as beta-lactamase inhibitors and antibacterial agents
INVENTOR(S): Musicki, Branislav
PATENT ASSIGNEE(S): Aventis Pharma SA, Fr.
SOURCE: Fr. Demande, 67 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2844273	A1	20040312	FR 2002-10957	20020905
WO 2004022563	A1	20040318	WO 2003-FR2639	20030904
W: AE, AG, AL, AU, BA, BB, BR, BZ, CA, CN, CO, CR, CU, DM, DZ, EC, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NI, NO, NZ, OM, PG, PH, PL, RO, SC, SG, SY, TN, TT, UA, UZ, VC, VN, YU, ZA				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004097490	A1	20040520	US 2003-655364	20030904
EP 1537117	A1	20050608	EP 2003-769564	20030904
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006501258	T2	20060112	JP 2004-533566	20030904
PRIORITY APPLN. INFO.:			FR 2002-10957 A	20020905
			WO 2003-FR2639 W	20030904

OTHER SOURCE(S): MARPAT 140:235731
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

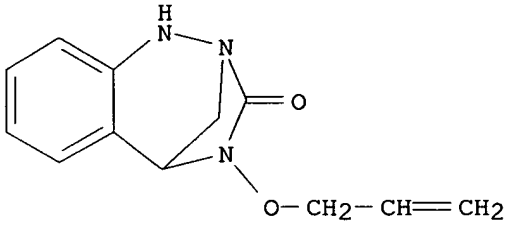
AB Title compds. I [wherein Y = (CH2)n; n = 1 or 2; R1 = H, alkyl, (CH2)mR'; m = o or 1; R' = heteroaryl/aryl; R2 = H, halo, alkyl, OH and derivs., NO2, alkylaminocarbonyl/alkylsulfonyl/alkylcarbonylmonoalkyl/dialkyl/amino , alkylaminocarbonyl, alkylaminosulfonyl, CO2H and derivs., CN, alkylsulfonyloxy, alkylcarbonyl, alkyl; X = -C(:O)-N(OH)- and derivs.] were prepared as beta-lactamase inhibitors and antibacterial agents. For example, II was prepared by cyclization of 2-acetylaniline in the presence of NaNO2/HCl, oxidation of cinnolinol, mono-Boc protection at the 2-position, oxidation of cinnolinone with O-(allyl)hydroxyamine, reduction of the O-alkylated oxime, Boc-deprotection, and cyclization of III•2HCl with diphosgene in the presence.of MeCN/TEA/DMAP. Selected I were able to inhibit either TEM-1 (enzyme from Escherichia coli) and P99 (enzyme from E. Cloacae) with IC50 values in the range of 0.012 mM to 0.57 mM and 0.015 to 0.46 mM, resp., when tested in competition expts. using nitrocefin as the reporter substrate. I were tested against two Gram-pos. bacteria as well as four Gram-neg. bacteria. Thus, I are and their compns. with β-lactam antibiotics, are useful as beta-lactamase inhibitors and

antibacterial agents.

IT **667467-63-2P 667467-74-5P**, 2-Propenyl [(3-oxo-2,3,4,5-tetrahydro-2,5-methano-1H-1,2,4-benzotriazepin-4-yl)oxy]acetate **667467-79-0P 667467-82-5P 667467-85-8P 667467-88-1P 667467-91-6P 667467-92-7P 667467-93-8P 667468-03-3P 667468-04-4P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(antibacterial agent; preparation of cinnolines as beta-lactamase inhibitors and anti-bacterial agents)

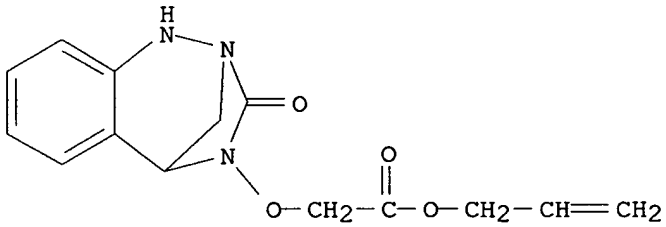
RN 667467-63-2 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepin-3(1H)-one, 4,5-dihydro-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)



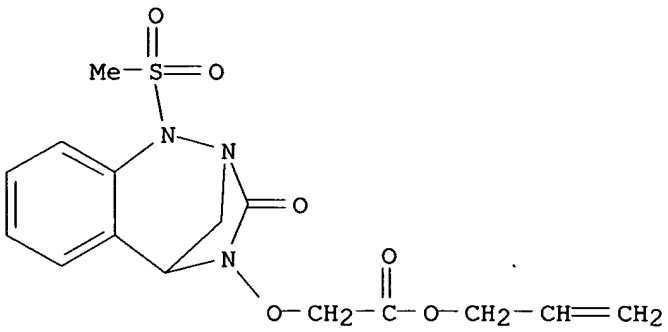
RN 667467-74-5 CAPLUS

CN Acetic acid, [(1,5-dihydro-3-oxo-2,5-methano-2H-1,2,4-benzotriazepin-4(3H)-yl)oxy]-, 2-propenyl ester (9CI) (CA INDEX NAME)

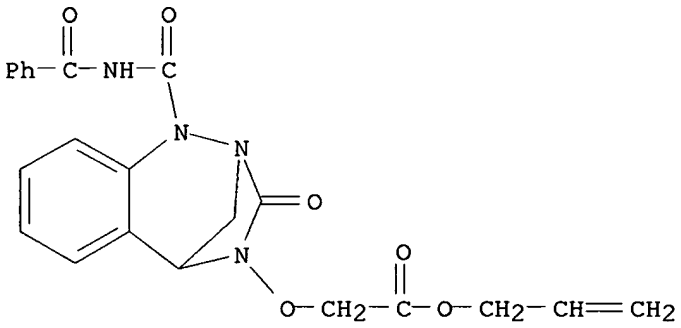


RN 667467-79-0 CAPLUS

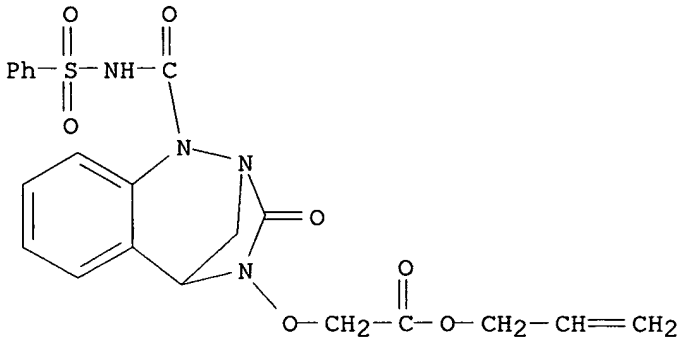
CN Acetic acid, [[1,5-dihydro-1-(methylsulfonyl)-3-oxo-2,5-methano-2H-1,2,4-benzotriazepin-4(3H)-yl]oxy]-, 2-propenyl ester (9CI) (CA INDEX NAME)



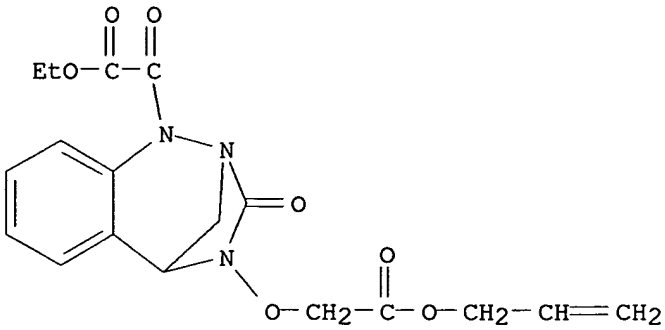
RN 667467-82-5 CAPLUS
CN Acetic acid, [[1-[(benzoylamino)carbonyl]-1,5-dihydro-3-oxo-2,5-methano-2H-1,2,4-benzotriazepin-4(3H)-yl]oxy]-, 2-propenyl ester (9CI) (CA INDEX NAME)



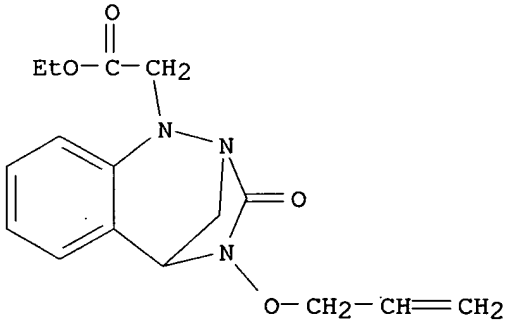
RN 667467-85-8 CAPLUS
CN Acetic acid, [[1,5-dihydro-3-oxo-1-[[(phenylsulfonyl)amino]carbonyl]-2,5-methano-2H-1,2,4-benzotriazepin-4(3H)-yl]oxy]-, 2-propenyl ester (9CI) (CA INDEX NAME)



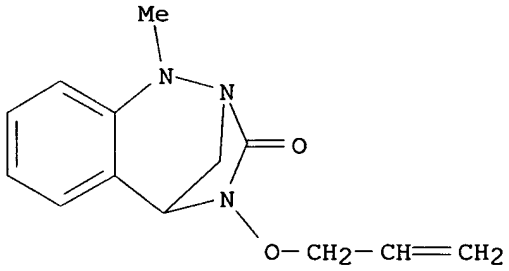
RN 667467-88-1 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-acetic acid, 1,3,4,5-tetrahydro-α,3-dioxo-4-[2-oxo-2-(2-propenyloxy)ethoxy]-, ethyl ester (9CI) (CA INDEX NAME)



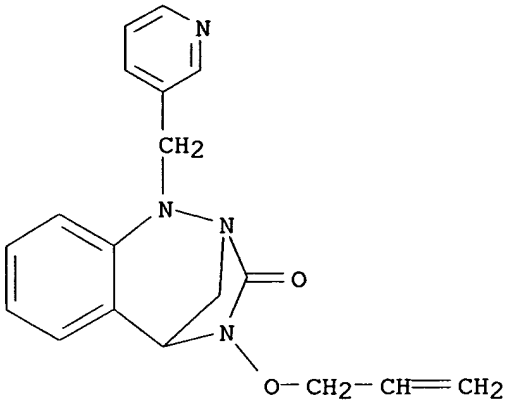
RN 667467-91-6 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-acetic acid, 1,3,4,5-tetrahydro-3-oxo-4-(2-propenyloxy)-, ethyl ester (9CI) (CA INDEX NAME)



RN 667467-92-7 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepin-3(1H)-one, 4,5-dihydro-1-methyl-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)

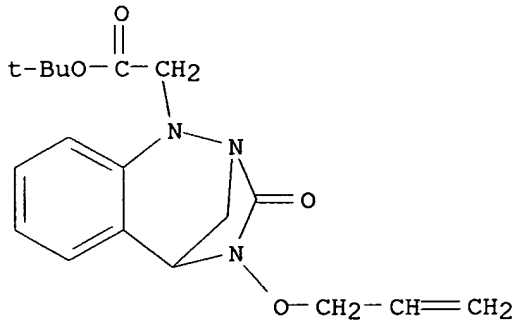


RN 667467-93-8 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepin-3(1H)-one, 4,5-dihydro-4-(2-propenyloxy)-1-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

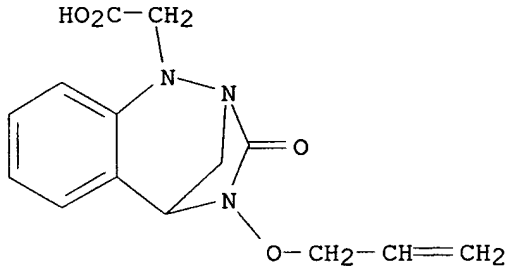


6

RN 667468-03-3 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-acetic acid, 1,3,4,5-tetrahydro-3-oxo-4-(2-propenyloxy)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



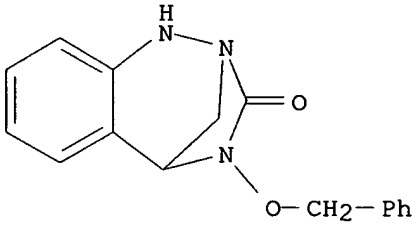
RN 667468-04-4 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-acetic acid, 1,3,4,5-tetrahydro-3-oxo-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)



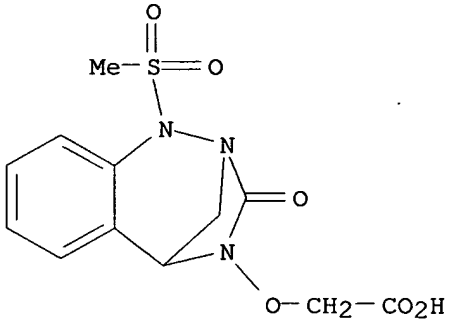
IT **667467-70-1P 667467-80-3P 667467-81-4P**
667467-83-6P 667467-84-7P 667467-86-9P
667467-87-0P 667467-89-2P 667467-90-5P
667467-94-9P 667467-95-0P 667467-96-1P
667467-97-2P 667467-98-3P 667467-99-4P
667468-00-0P 667468-01-1P 667468-02-2P

667468-05-5P 667468-06-6P 667468-07-7P
667468-08-8P 667468-09-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(antibacterial agent; preparation of cinnolines as beta-lactamase inhibitors and anti-bacterial agents)

RN 667467-70-1 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepin-3(1H)-one, 4,5-dihydro-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)



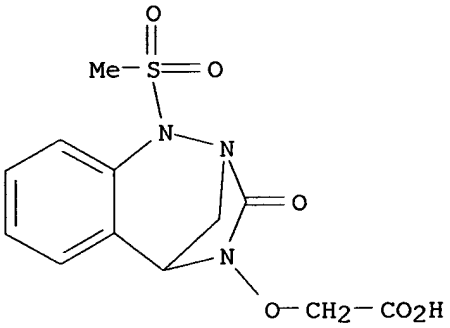
RN 667467-80-3 CAPLUS
CN Acetic acid, [[1,5-dihydro-1-(methylsulfonyl)-3-oxo-2,5-methano-2H-1,2,4-benzotriazepin-4(3H)-yl]oxy]- (9CI) (CA INDEX NAME)



RN 667467-81-4 CAPLUS
CN Acetic acid, [[1,5-dihydro-1-(methylsulfonyl)-3-oxo-2,5-methano-2H-1,2,4-benzotriazepin-4(3H)-yl]oxy]-, compd. with N-(1-methylethyl)-2-propanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 667467-80-3
CMF C12 H13 N3 O6 S

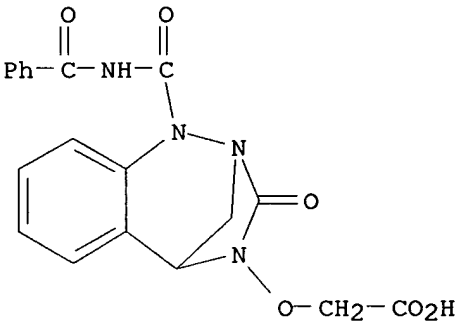


CM 2

CRN 108-18-9
CMF C6 H15 N

i-Pr—NH—Pr-i

RN 667467-83-6 CAPLUS
CN Acetic acid, [[1-[(benzoylamino)carbonyl]-1,5-dihydro-3-oxo-2,5-methano-2H-1,2,4-benzotriazepin-4(3H)-yl]oxy]- (9CI) (CA INDEX NAME)

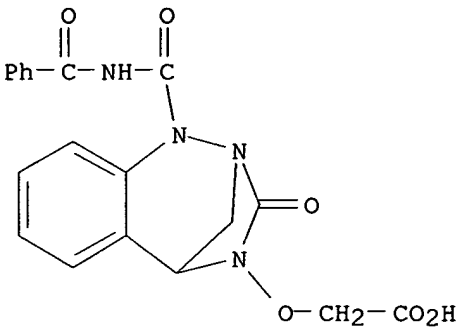


2

RN 667467-84-7 CAPLUS
CN Acetic acid, [[1-[(benzoylamino)carbonyl]-1,5-dihydro-3-oxo-2,5-methano-2H-1,2,4-benzotriazepin-4(3H)-yl]oxy]-, compd. with N-(1-methylethyl)-2-propanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 667467-83-6
CMF C19 H16 N4 O6

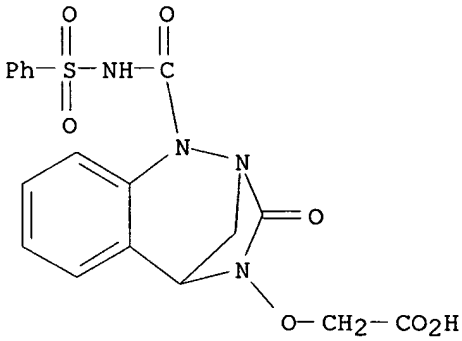


CM 2

CRN 108-18-9
CMF C6 H15 N

i-Pr—NH—Pr-i

RN 667467-86-9 CAPLUS
CN Acetic acid, [[1,5-dihydro-3-oxo-1-[[(phenylsulfonyl)amino]carbonyl]-2,5-methano-2H-1,2,4-benzotriazepin-4(3H)-yl]oxy]- (9CI) (CA INDEX NAME)

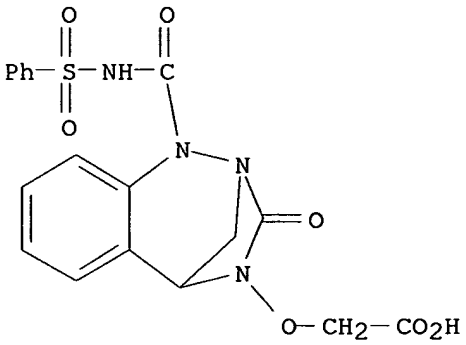


3

RN 667467-87-0 CAPLUS
CN Acetic acid, [[1,5-dihydro-3-oxo-1-[[(phenylsulfonyl)amino]carbonyl]-2,5-methano-2H-1,2,4-benzotriazepin-4(3H)-yl]oxy]-, compd. with N-(1-methylethyl)-2-propanamine (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 667467-86-9
CMF C18 H16 N4 O7 S

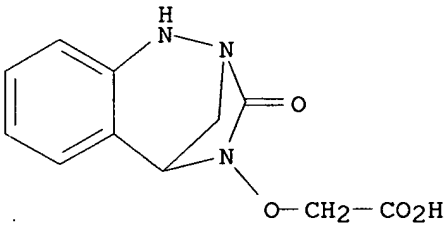


CM 2

CRN 108-18-9
CMF C6 H15 N

i-Pr—NH—Pr-i

RN 667467-89-2 CAPLUS
CN Acetic acid, [(1,5-dihydro-3-oxo-2,5-methano-2H-1,2,4-benzotriazepin-4(3H)-yl)oxy]- (9CI) (CA INDEX NAME)

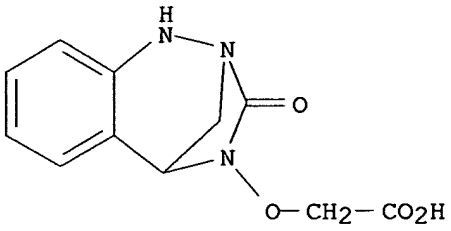


4

RN 667467-90-5 CAPLUS
CN Acetic acid, [(1,5-dihydro-3-oxo-2,5-methano-2H-1,2,4-benzotriazepin-4(3H)-yl)oxy]-, compd. with N-(1-methylethyl)-2-propanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 667467-89-2
CMF C11 H11 N3 O4

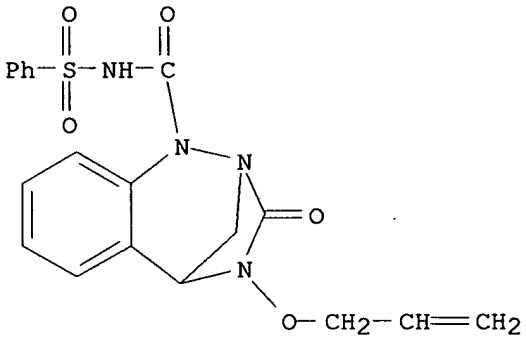


CM 2

CRN 108-18-9
CMF C6 H15 N

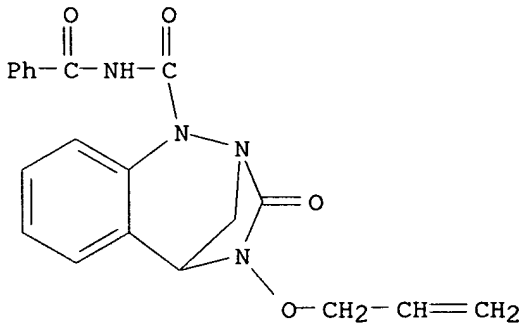
i-Pr—NH—Pr-i

RN 667467-94-9 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-carboxamide, 1,3,4,5-tetrahydro-3-oxo-N-(phenylsulfonyl)-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)



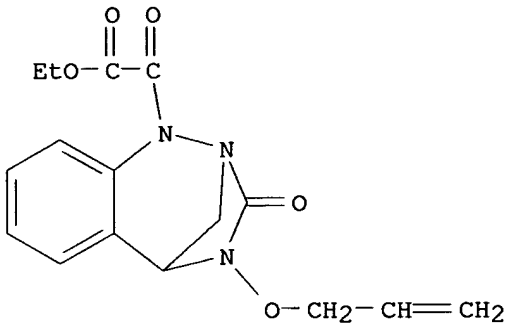
7

RN 667467-95-0 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-carboxamide, N-benzoyl-1,3,4,5-tetrahydro-3-oxo-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)



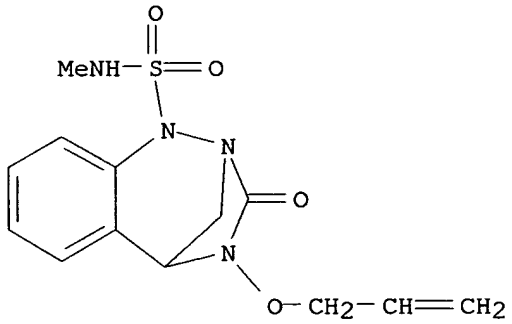
8

RN 667467-96-1 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-acetic acid, 1,3,4,5-tetrahydro-α,3-dioxo-4-(2-propenyloxy)-, ethyl ester (9CI) (CA INDEX NAME)

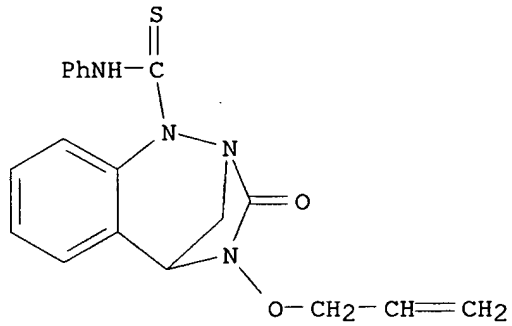


9

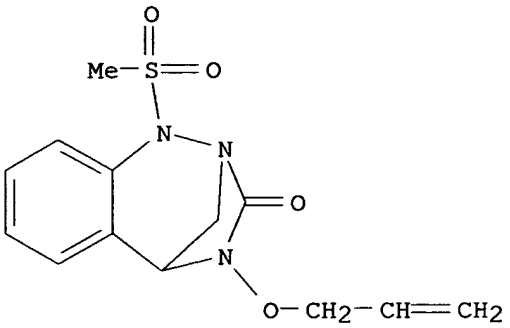
RN 667467-97-2 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-sulfonamide, 1,3,4,5-tetrahydro-N-methyl-3-oxo-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)



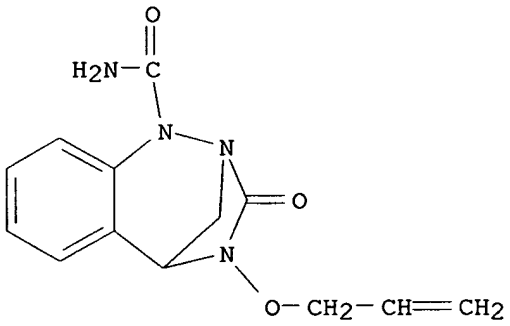
RN 667467-98-3 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-carbothioamide, 1,3,4,5-tetrahydro-3-oxo-N-phenyl-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)



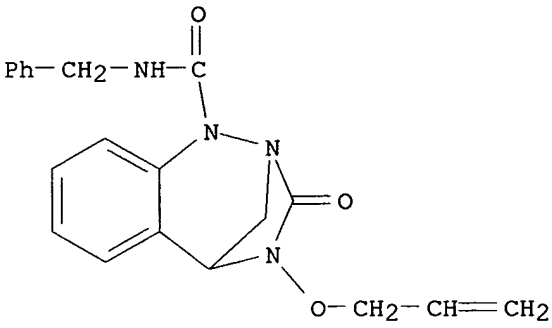
RN 667467-99-4 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepin-3(1H)-one, 4,5-dihydro-1-(methylsulfonyl)-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)



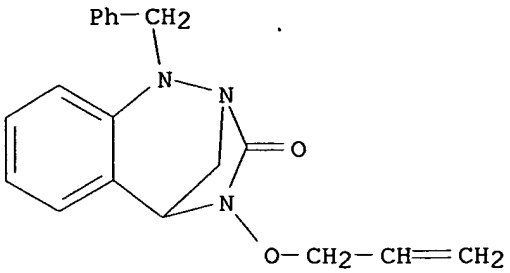
RN 667468-00-0 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-carboxamide, 1,3,4,5-tetrahydro-3-oxo-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)



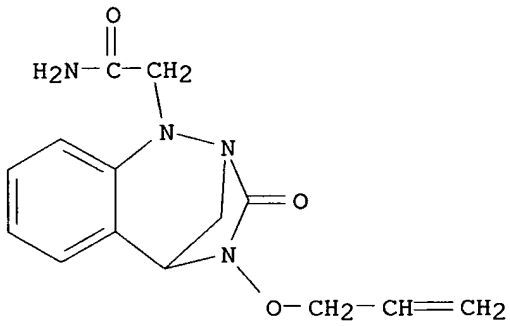
RN 667468-01-1 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-carboxamide, 1,3,4,5-tetrahydro-3-oxo-N-(phenylmethyl)-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)



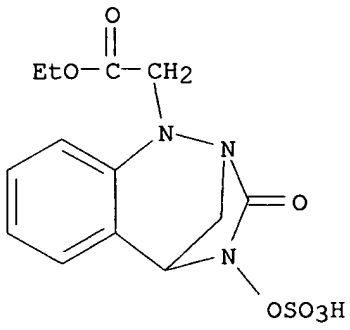
RN 667468-02-2 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepin-3(1H)-one, 4,5-dihydro-1-(phenylmethyl)-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)



RN 667468-05-5 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-acetamide, 1,3,4,5-tetrahydro-3-oxo-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)

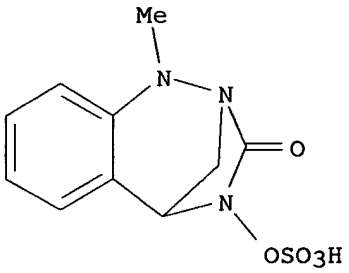


RN 667468-06-6 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-acetic acid, 1,3,4,5-tetrahydro-3-oxo-4-(sulfooxy)-, α-ethyl ester, sodium salt (9CI) (CA INDEX NAME)



● Na

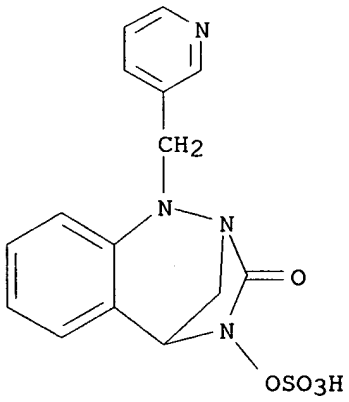
RN 667468-07-7 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepin-3(1H)-one, 4,5-dihydro-1-methyl-4-(sulfooxy)-, sodium salt (9CI) (CA INDEX NAME)



5

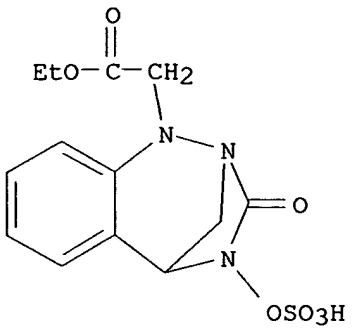
● Na

RN 667468-08-8 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepin-3(1H)-one, 4,5-dihydro-1-(3-pyridinylmethyl)-4-(sulfooxy)-, sodium salt (9CI) (CA INDEX NAME)



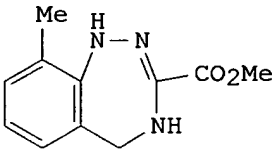
● Na

RN 667468-09-9 CAPLUS
CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-acetic acid, 1,3,4,5-tetrahydro-3-oxo-4-(sulfooxy)-, α-ethyl ester (9CI) (CA INDEX NAME)

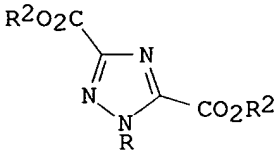


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

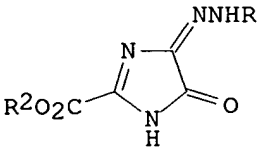
L6 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:77053 CAPLUS
DOCUMENT NUMBER: 112:77053
TITLE: Thermally induced fragmentation and cyclization of C-azidohydrazones
AUTHOR(S): Bruche, Luca; Garanti, Luisa; Zecchi, Gaetano
CORPORATE SOURCE: Dip. Chim. Org. Ind., Univ. Milan, Milan, 20133, Italy
SOURCE: Journal of Heterocyclic Chemistry (1989), 26(3), 619-24
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:77053
GI



II



III



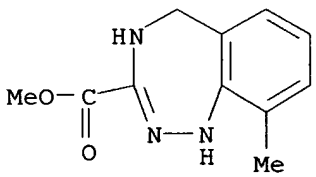
IV

AB C-Azidohydrazones RNHN:CR1CO2R2 (I, R = Ph, 4-MeC6H4, 3,5-Me2C6H3, 2,6-Me2C6H3, 2-MeC6H4, R2 = Me; R = 2-NCC6H4, R2 = Et; R1 = N3) were synthesized from the corresponding C-chlorohydrazones I (R, R2 = same; R1 = Cl) and submitted to thermal decomposition in boiling C6H6. Various kinds of products were obtained due to competitive modes of evolution of first-formed nitrenes I (R1 = N•), namely H abstraction to form aminohydrazones I (R1 = NH2) and benzotriazepine II and radical fragmentation to give diaryls RPh and arylglyoxylate arylhydrazones RNHN:CRCO2R2. Ring-closed products, namely 1,2,4-triazoles III and imidazolones IV were also formed.

IT **125240-53-1P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in thermal decomposition of azidohydrazone)

RN 125240-53-1 CAPLUS

CN 1H-1,2,4-Benzotriazepine-3-carboxylic acid, 2,5-dihydro-9-methyl-, methyl ester (9CI) (CA INDEX NAME)



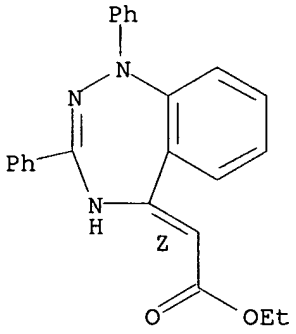
L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:75084 CAPLUS
DOCUMENT NUMBER: 94:75084
TITLE: Crystal structure of 1,3-diphenyl-5-carbethoxymethylene-1H-4,5-dihydro-1,2,4-benzotriazepine
AUTHOR(S): Perez-Salazar, A.; Cano, F. H.; Garcia-Blanco, S.
CORPORATE SOURCE: Inst. Quim. Fiz. "Rocasolano", CSIC, Madrid, 6, Spain
SOURCE: Journal of Crystal and Molecular Structure (1980), Volume Date 1979, 9(6), 317-23
CODEN: JCMLB5; ISSN: 0308-4086
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The title compound is orthorhombic, space group P212121, with a 15.1342(3), b 14.1692(3), and c 9.6533(3) Å; d.(exptl.) = 1.23 and Z = 4. The structure was solved by direct methods and refined to R 0.048 (Rw = 0.068) for 1831 observed reflections. An intramol. H bond is present. The conformation of the 7-membered ring is boatlike with a quasi-mirror plane through N(1).

IT **76553-23-6**
RL: PRP (Properties)
(crystal structure of)

RN 76553-23-6 CAPLUS
CN Acetic acid, (1,2-dihydro-1,3-diphenyl-5H-1,2,4-benzotriazepin-5-ylidene)-, ethyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L6 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1980:198370 CAPLUS
DOCUMENT NUMBER: 92:198370
TITLE: Studies on 7-membered benzo condensed heterocycles. 6. 5-Oxo-1H-4,5-dihydro-1,2,4-benzotriazepines. Chemical behavior towards alkylating, acidic and alkaline agents
AUTHOR(S): Bianchi, Mario; Hausermann, Enrico; Rossi, Silvano
CORPORATE SOURCE: Dep. Chem., Roussel Maestretti S.p.A., Milan, 20131, Italy
SOURCE: Journal of Heterocyclic Chemistry (1979), 16(7), 1411-16
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 92:198370

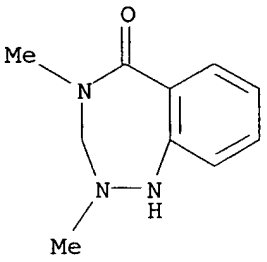
AB The chemical behavior of 4-methyl- and 4-phenyl-5-oxo-1H-4,5-dihydro-1,2,4-benzotriazepines towards methylating and acidic agents was studied. The 4-Me derivative, when treated with FSO3Me furnished, after crystallization from H2O, a quaternary salt (2,4-dimethyl-5-oxo-1H-4,5-dihydro-1,2,4-benzotriazepinium fluorosulfonate); from the 4-Ph derivative a complex mixture was obtained, which, after boiling with H2O, afforded 2-methylindazolone, PhNH2.HO3SF and HCO2H. In acidic medium the 4-Me derivative isomerized to 1-imino-3-methylquinazolin-4-one, but the 4-Ph derivative exclusively yielded products resulting from ring opening. In alkaline medium, both compds. gave hydrolytic cleavage products.

IT **73647-13-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of)

RN 73647-13-9 CAPLUS
CN 1H-1,2,4-Benzotriazepinium, 4,5-dihydro-2,4-dimethyl-5-oxo-, fluorosulfate (9CI) (CA INDEX NAME)

CM 1

CRN 73647-12-8
CMF C10 H12 N3 O



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 15181-47-2
CMF F O3 S